Statistical fluctuations for the fission process on its decent from saddle to scission

H. Hofmann *†
Physik-Department, TU München, D-85747 Garching
and
D. Kiderlen
National Superconducting Cyclotron Laboratory
Michigan State University, East Lansing, Michigan 48824
Physik-Department, TU München, D-85747 Garching

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Abstract

We reconsider the importance of statistical fluctuations for fission dynamics beyond the saddle in the light of recent evaluations of transport coefficients for average motion. The size of these fluctuations are estimated by means of the Kramers-Ingold solution for the inverted oscillator, which allows for an inclusion of quantum effects.

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Kramers' transport equation [1] delivers the classic description of the dynamics of fission at finite excitation. It restricts to the high temperature regime in which collective motion is

*e-mail: hhofmann@.physik.tu-muenchen.de
†http://www.physik.tu-muenchen.de/tumphy/e/T36/hofmann.html

treated within the frame of classical statistical mechanics. An extension to the quantum case has been described in [2], [3] and [4]. This is possible within a locally harmonic approximation, in which global motion is described in terms of local propagators. The latter are constructed as special solutions of an appropriate transport equation in which anharmonic forces are linearized around some given point in phase space [6]. For the present purpose this equation is needed only for the region between barrier and scission point. To simplify matters we like to apply the schematic model of [5], in which the potential is represented by an inverted oscillator (centered at $q = 0$) and where the coefficients for inertia M and friction γ do not change along the fission path. The transport equation for the distribution $d(q, P, t)$ in collective phase space may then be written as:

$$\frac{\partial}{\partial t} d(q,P,t) = \left[-\frac{\partial}{\partial q}\frac{P}{M} + \frac{\partial}{\partial P} Cq + \frac{\partial}{\partial P}\gamma\frac{P}{M} + D_{qp}\frac{\partial^2}{\partial q \partial P} + D_{pp}\frac{\partial^2}{\partial P \partial P} \right] d(q,P,t) \tag{1}$$

with C being the (negative) stiffness coefficient. There is little doubt that a correct treatment would require to go beyond the harmonic approximation underlying the form (1). Not only that the potential energy along the fission path will, in general, be more complicated than given by the simple quadratic dependence $Cq^2/2$. Also the other transport coefficients will vary with q. However, recent numerical computations [7], [8] have revealed that the following ratios

$$\varpi = \sqrt{\frac{\mid C \mid}{M}} \qquad\qquad \eta = \frac{\gamma}{2M\varpi} \tag{2}$$

are quite stable. As we shall see soon, within the harmonic approximation it is them which parameterize the quantities we are mostly interested in, namely the kinetic energy and its fluctuation.

As compared to the form of Kramers' equation, only two modifications occur in (1), both referring to the diffusive terms. Firstly, there appears a cross term with the D_{qp} being different from zero in the quantal regime. Secondly, the coefficient D_{pp} will be given by the classic Einstein relation $D_{pp} = \gamma T$ only at large temperatures when quantum effects disappear. In their quantum version, these coefficients are defined by the following expressions

$$D_{pp} = \gamma M \int_{\mathcal{C}} \frac{\mathrm{d}\omega}{2\pi}\, \hbar \coth\left(\frac{\hbar\omega}{2T}\right) \chi''_{qq}(\omega)\, \omega^2 \equiv \frac{\gamma}{M}\Sigma^{\mathrm{eq}}_{pp} \tag{3}$$

$$D_{qp} = \int_{\mathcal{C}} \frac{\mathrm{d}\omega}{2\pi}\, \hbar \coth\left(\frac{\hbar\omega}{2T}\right) \chi''_{qq}(\omega) \left[C - M\omega^2\right] \equiv C\Sigma^{\mathrm{eq}}_{qq} - \frac{1}{M}\Sigma^{\mathrm{eq}}_{pp} \tag{4}$$

They are a consequence of the fluctuation dissipation theorem (FDT): Together with some simple symmetry relations, it allows one to calculate the "equilibrium fluctuations" $\Sigma^{\mathrm{eq}}_{qq}$ and $\Sigma^{\mathrm{eq}}_{pp}$ from the dissipative part $\chi''_{qq}(\omega)$ of the response function which represents average motion in $q(t)$. For the linearized version used here, the latter must be related to the one of a damped

oscillator determined by M, γ and C. If (1) is applied to a bound oscillator with $C > 0$, the expressions (3, 4) warrant that for $t \to \infty$ the dynamical fluctuations in q, P turn into those of equilibrium as determined by the FDT [2]. Thus the contour $\mathcal{C}$ has to be chosen in the common way, namely along the real axis extending from $-\infty$ to ∞. For unbound motion with $C < 0$, the case we want to study here, one has to apply suitable analytical continuations. This is possible in two ways: (i) One may evaluate the forms given in (3, 4) for $C > 0$ and perform the continuations in the expressions one obtains after performing the integration (see [3] and [4]). (ii) In an alternative method [10] one redefines the contour $\mathcal{C}$. This allows for more general applications like in [11]. For more details we refer to [9] and [6].

With respect to the evaluation of (3, 4) we need to clarify a problem hidden in the integrals. In the quantum regime, some of them would diverge if we one were to take for the response function that of the damped oscillator. This problem is well known, and one possible solution is to apply the Drude regularization. This means to replace the $\chi_{qq}(\omega)$ by

$$\chi_D(\omega) = \frac{1}{-M\omega^2 - i\gamma(\omega)\omega + C} \tag{5}$$

with a frequency dependent friction coefficient

$$\frac{\gamma_D(\omega)}{\gamma} = \left(1 - i\frac{\omega}{\varpi_D}\right)^{-1} \tag{6}$$

In this way a "cut-off" frequency ω_D is introduced. We do not want to discuss the interesting questions of how its value can be fixed and from which physical quantities. For the computations to be discussed below we chose $\omega_D = 10\varpi$, with the ϖ given by (2). Fortunately, the diffusion coefficients do not depend on ω_D too much (see [9]). Changing the latter by a factor of two, our final results would have to be modified by less than 30% which, as we shall see, will not influence much the conclusions we are going to draw below.

Notice, please, that this regularization problem disappears in the classical limit. The latter is obtained if the $\hbar \coth(\hbar\omega/(2T))$ is replaced by $2T/\omega$. With such a weighting factor all integrals in (3) and (4) converge even for the case of a constant friction force. Apparently this classical limit is identical to the high temperature limit, for which one needs to have $\hbar\omega \ll T$. Looking back to the right hand sides of (3) and (4), it becomes evident why in this case the diffusion coefficients turn into those of Kramers' equation. For stable modes this is simply a consequence of the (classical) equipartition theorem. Since the diffusion coefficients then become independent of C the analytic continuation is trivial, and does not change the results for D_{pp} and D_{qp} when turning to the unstable situation.

Whereas for stable modes the extension of Kramers' equation to the quantum regime is possible for all temperatures and all possible values of the transport coefficients, for unstable ones the description ceases to make sense at very low temperatures. First of all, below a

certain T_0 it is not possible anymore to save the integral representation of the FDT. The contour $\mathcal{C}$ needs to cross the imaginary axis between the pole $\omega_+ = i \mid \omega_+ \mid$ of the unstable mode and the first Matsubara frequency $\omega_M^1 = 2\pi T/\hbar$ (see [9]-[11]). The T_0 obtained in this way, namely $T_0 = \hbar\omega_+ \mid /(2\pi)$, is identical to the so called "cross over" temperature known from treatments of "dissipative tunneling" with functional integrals in the imaginary time domain. Here we are looking at real time propagation for which in a model case Ingold [12] has been able to construct a phase space distribution corresponding to a constant flux across the barrier. Such a construction is possible above a critical temperature $T_c > T_0$. As shown in [3] this distribution solves the transport equation (1) if only the diffusion coefficients are defined as described above. In this sense it may be considered the generalization to the quantum regime of the stationary solution found by Kramers. Actually, this T_c turns out to be that temperature at which the $C\Sigma_{qq}^{\rm eq}$ becomes negative. It is of the order of 0.5 MeV or less, depends on the transport coefficients of average motion and decreases with increasing damping, see [9]. On the nuclear scale such values of T can be considered small. (As a matter of fact, in such a regime the very concept of temperature itself becomes questionable.) Commonly, the fission experiments, which one may want to interpret with such a transport equation, involve higher excitations, for which our extension thus applies. Unfortunately, an experimental verification of the existence of quantum effects is still missing. Two possibilities have been suggested so far, the (dwell) time τ from saddle to scission [3] (see below), and the decay rate [4]. For those, however, quantum effects would show up only in a very narrow range between T_c and values of about $T \simeq 1 \cdots 1.5$ MeV.

This situation may change if one looks at quantities which involve the momentum distribution. Such a feature is known from studies of the dynamics of *stable modes*. There the equilibrium fluctuations in the coordinate get squeezed when friction increases. In this way their values get *closer* to the *classical* limit. The opposite holds true for the momentum. A nice demonstration of this effect can be found in [13] where path integrals are applied to a solvable model. In [9] this problem has been taken up for the nuclear context within the locally harmonic approximation, for which one is not restricted to describe the "heat bath" of the nucleonic degrees of freedom by a set of coupled oscillators.

In the present letter we specifically address the dynamics across the fission barrier. Different to [3] and [4] we want to exploit the Kramers-Ingold solution $d_I(q,P)$ to evaluate the kinetic energy and its variance at scission. The calculation can be done in complete analogy to the case discussed in [5] for Kramers' equation. The average kinetic energy at scission may be defined by

$$E_{\rm kin} = \int_{-\infty}^{\infty} \frac{P\,dP}{Mj}\, d_I(q_{sc},P)\, \frac{P^2}{2M} \tag{7}$$

and its variance by

$$\sigma^2_{\rm kin} = \int_{-\infty}^{\infty} \frac{P\,dP}{Mj}\; d_I(q_{sc},P)\, \left(\frac{P^2}{2M}\right)^2 \quad - \quad (E_{\rm kin})^2\,. \tag{8}$$

with the q_{sc} being the coordinate of the scission point. Notice please, that the sampling is done for the following normalization of the distribution

$$\int_{-\infty}^{\infty} \frac{P\,dP}{Mj}\; d_I(q,P) = 1 \tag{9}$$

with j being the constant flux across the barrier. Like in the classical case (see eqs.(13) and (14) of [5]) the integrals can be carried out analytically. Introducing the abbreviation

$$\zeta = \sqrt{1+\eta^2} - \eta \equiv \frac{1}{\sqrt{1+\eta^2}+\eta} \tag{10}$$

the result writes as

$$E_{\rm kin} = \frac{1}{2}\left(M\varpi^2 q^2_{sc} - D_{qp}\right)\zeta^2 + \frac{D_{pp}}{\gamma}\,(1+\eta\zeta) \tag{11}$$

and

$$\sigma^2 = \left(\frac{D_{pp}}{\gamma}\right)^2 + \frac{1}{2}\zeta^2\left[\left(2\eta\frac{D_{pp}}{\gamma} - \zeta D_{qp} + M\varpi^2 q^2_{sc}\zeta\right)^2 - (M\varpi^2 q^2_{sc}\zeta)^2\right] \tag{12}$$

For the difference $\Delta V = \frac{1}{2}M\varpi^2 q^2_{sc}$ of the potential energy between saddle and scission the value $\Delta V = 20$ MeV will be adopted in the following. Notice please, that the first term in (11) stands for the kinetic energy $E^{\rm traj}_{\rm kin} = M\varpi^2 q^2_{sc}\zeta^2/2$ one would obtain in a mere trajectory calculation. This is easily verified from the solution

$$q_{sc} = q(\tau) \approx \frac{P_0}{2M\varpi\sqrt{1+\eta^2}}\exp(\varpi(\sqrt{1+\eta^2}-\eta)\tau) \tag{13}$$

of Newton's equation for $q(t=0)=0$, only assuming the saddle to scission time τ to be sufficently large to have $\varpi\sqrt{1+\eta^2}\tau \gg 1$. In (11) all the other terms represent the effects of the fluctuating force.

Before turning to discuss numerical evaluations of the expressions just presented it may be worth while to comment on their physical relevance. Firstly, we like to stress that by using the stationary solution $d_I(q,P)$ the results become *insensitive* to initial conditions, like those on top of the barrier one would need to invoke in a time dependent picture. Please notice that the only uncertainty left in $d_I(q,P)$ is the multiplicative factor hidden in the current j which drops out when calculating the $E_{\rm kin}$ and $\sigma^2_{\rm kin}$ according to (7) and (8), respectively. For the situation to which this stationary solution $d_I(q,P)$ of the inverted oscillator commonly is applied to (c.f.[1]), this j can be said to stand for the decay rate out of the potential miminum. Eventually, one would then like to have this minimum to be well pronounced, in the sense

of having the barrier height be large compared to T, more precisely to that temperature the system has on its way towards the saddle. However, as demonstrated in [14] and [15] the $d_I(q, P)$ may as well be understood to result from integrating a t-dependent distribution $d(q, P, t)$ over time t. It is not difficult to understand that such a time integrated function solves an equation like (1) with the left hand side put equal to zero. Moreover, as shown in [15], already for quite small damping rates η (called γ in [15]) this time-integrated distribution shows a relaxational behavior to Kramers solution, if considered in its dependence on q. In this spirit, formulas (7) to (12) may be understood in the following way. Provided that the scission point q_{sc} does not lie too closely to the position of the barrier top, we may assume the $d_I(q, P)$ to adequately portray the momentum distribution of an actual fission process. Formulas (11) and (12) then measure the kinetic energy and its fluctuation for the distribution one obtains after summing up all events leading to fission.

In Fig.1 we show the kinetic energy as function of η for different temperatures as calculated from (11). Fully drawn lines correspond to the quantal case and dashed ones to the high

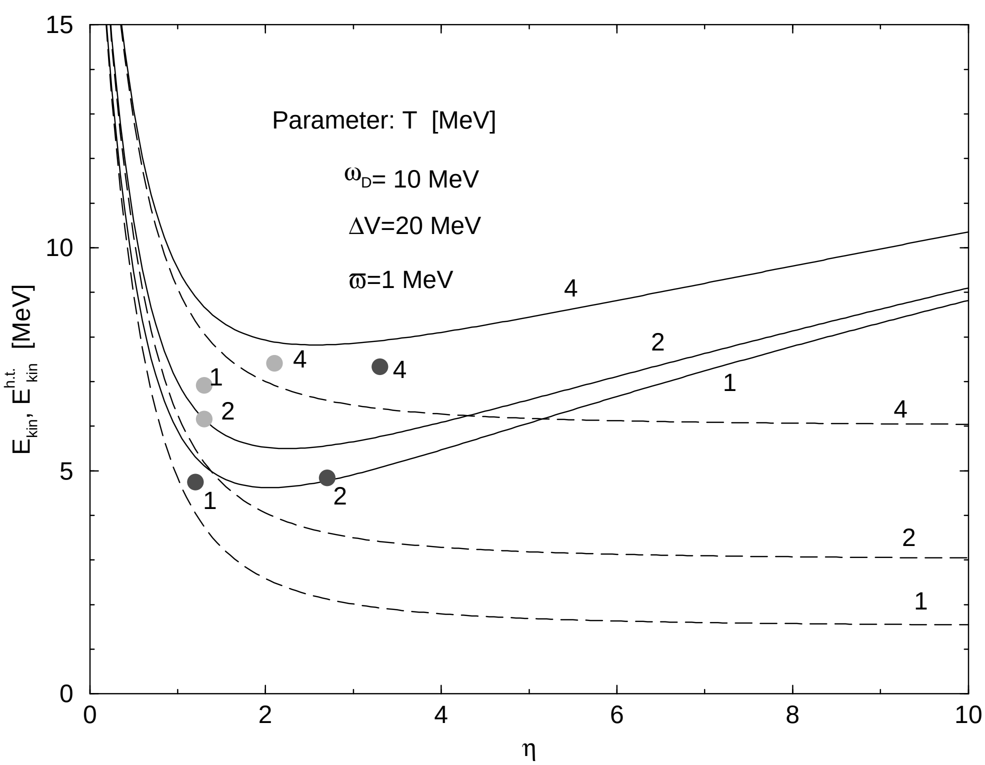

Figure 1: Average kinetic energy as function of η for different temperatures T. Fully drawn curves include quantum effects, dashed ones refer to Kramers' solution. Shaded dots give results based on the values for ϖ and η (at given T) as obtained in microscopic computations of [7](dark shaded) and [8](light shaded). (In this and the following figures we use units of $\hbar = 1$).

temperature limit, thus corresponding to Kramers' equation. As the figure demonstrates, quantum effects increase with damping and they amplify the average kinetic energy. As a matter of fact, the latter is seen to attain quite large values in any case, if compared to the value of ΔV. Obviously, this is an effect of the fluctuating force, as friction alone acts to diminish the velocity and thus the kinetic energy. This feature is demonstrated explicitly in Fig.2. There the ratio $E_{\rm kin}^{\rm traj}/E_{\rm kin}$ is shown (with the $E_{\rm kin}^{\rm traj}$ introduced below (12)). In both

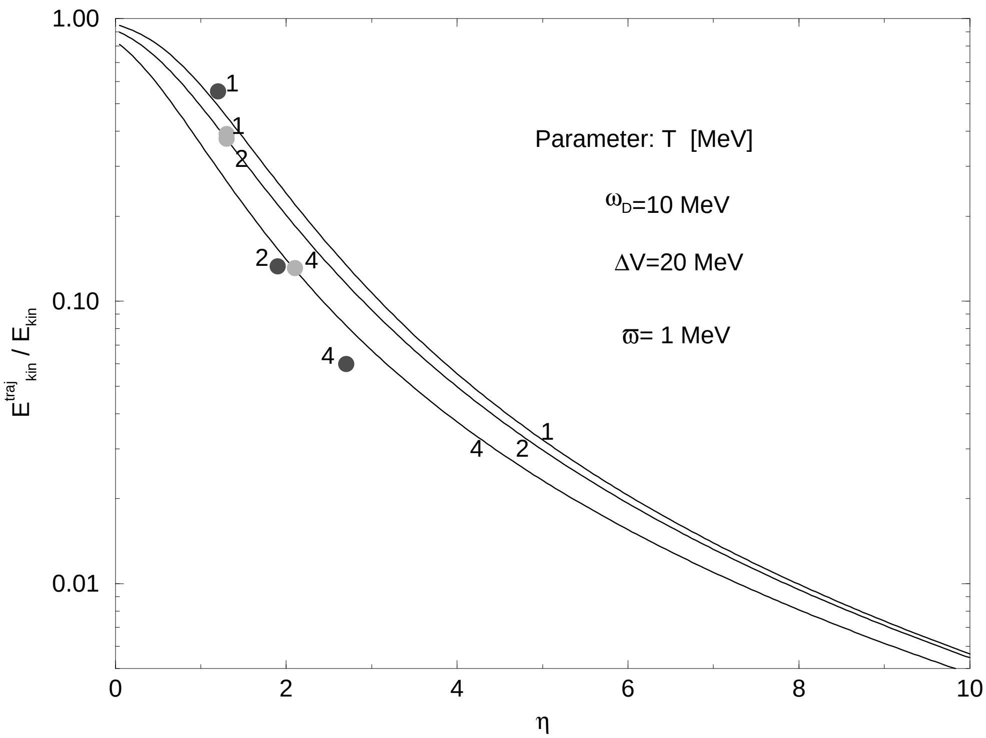

Figure 2: Ratio of the kinetic energies, $E_{\rm kin}^{\rm traj}$ and $E_{\rm kin}$, calculated, respectively, without and with fluctuating force. The dots are specified as in Fig.1.

figures shaded circles indicate results obtained by using the transport coefficients for average motion as found in microscopic computations of [7] (dark shaded) and [8] (light shaded). Fig.2 demonstrates clearly that trajectory calculations may grossly underestimate the size of $E_{\rm kin}$.

The very fact of the big influence of the fluctuating force hints at the importance of statistical fluctuations of the kinetic energy itself, which may be calculated according to (12). In Fig.3 we show the square root of the variance σ divided by the kinetic energy $E_{\rm kin}$, both calculated at the scission point. For large damping and large temperatures this ratio comes close to the limiting value $\sqrt{2/3}$. When the effective damping rate η is somewhat larger than 1 this value of $\sqrt{2/3}$ is reached for practically all T. Incidentally, we may note that this ratio $\sigma/E_{\rm kin}$ can be expected less sensitive to the Drude frequency ω_D than the individual

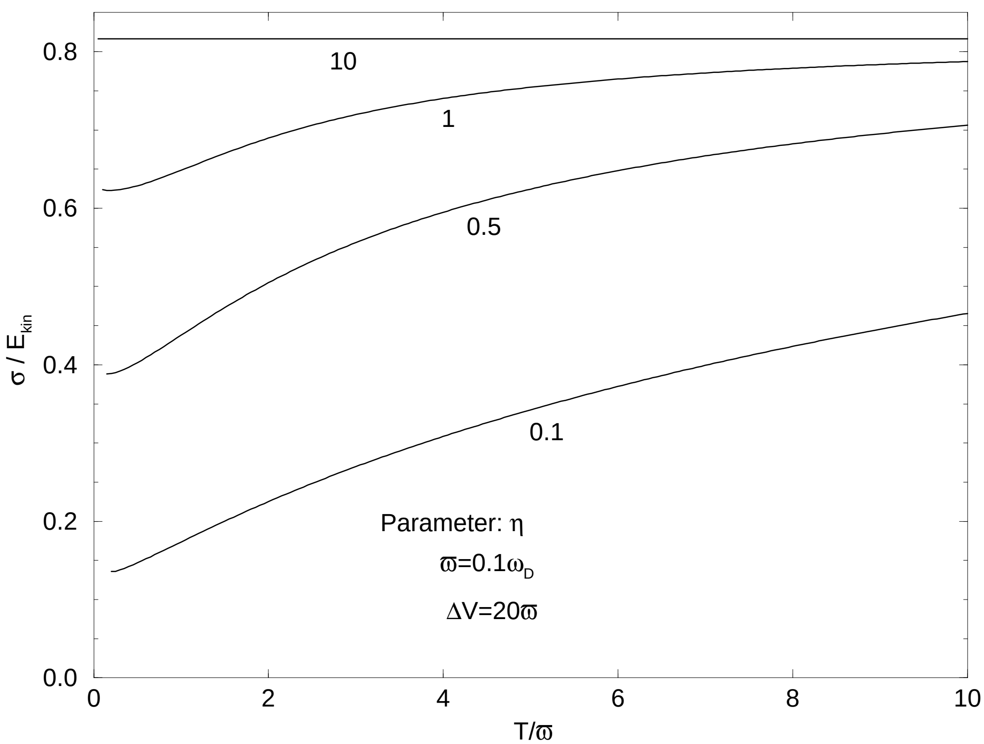

Figure 3: Variance σ over average kinetic energy $E_{\rm kin}$ as function of T/ϖ, for different values of η.

quantities, simply because both of the quantities, σ and $E_{\rm kin}$, change with ω_D alike.

Next we like to work out more explicitly the size of quantum effects. In Fig.4 we plot for both the kinetic energy and its fluctuations, the ratio of the values in the quantal case to the corresponding ones in the high-T limit (Kramers' case). As seen from the figure, these ratios may take on quite large values and they increase with increasing damping. Thus Fig.4 agrees with the observation made in Fig.1 and confirms our conjecture raised earlier: Whenever the collective momentum is involved quantum effects get larger with increasing damping. Like before we have again indicated by dots the range one would expect for these values on the basis of the microscopic computations of [7] and [8]. Notice, please, that in these computations the coefficients η and ϖ have been evaluated as function of T. For the curves shown in all the figures these coefficients have been varied as free parameters. This will facilitate comparison with other theoretical models and with results deduced from experiments. Indeed, it may be said that there is experimental evidence (see e.g. [16] and [17]) for much larger damping coefficients than found in [7] and [8]. The authors of [17] need values of as much as $\eta = 10$ to cope with findings in experiments where fission of heavy nuclei is observed accompanied by GDR γ rays, at temperatures not larger than about 2MeV. Applying macroscopic pictures to evaluate the transport coefficients, like the wall formula for friction, irrotational flow for

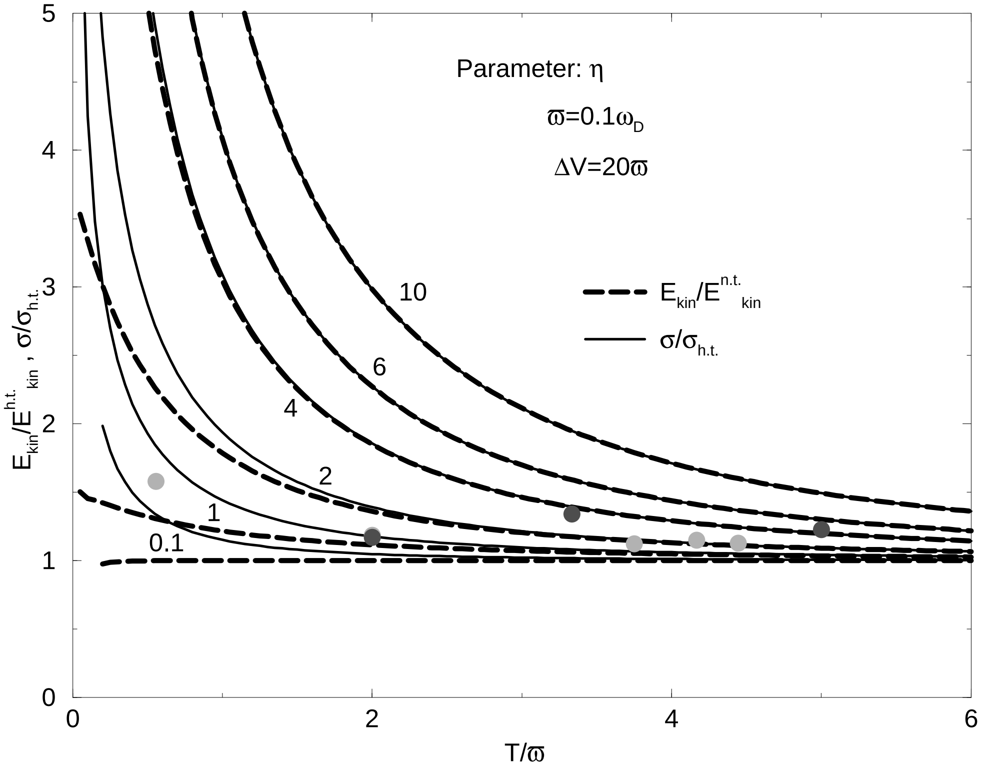

Figure 4: Ratios of kinetic energy and its variance to their values in the high temperature limit, both as functions of T/ϖ, again for different η.

inertia and the liquid drop model for the stiffness one would find similar values [18] (for ^{224}Th at $T = 2$ MeV η becomes ≈ 7.5). If one looks at lighter systems where large angular momenta are needed to find fission events with some finite chance [19], the barrier becomes quite small and broad, thus leading to smaller values of ϖ and hence to larger values of η [18]. As seen from our figures, this hints not only at the importance of the statistical fluctuations as such, but also at the necessity of calculating them with the quantal diffusion coefficients. Most likely this may again modify the interpretation of experimental results. In any case, it is probably fair to say that still some work is to be done before more conclusive statements can be made about the size of the transport coefficients. In this context one may mention that there are indications from other experiments that η might be smaller, indeed, than the macroscopic picture requires [20].

So far in this paper we have been looking at cases which explicitly involve the momentum distribution in one way or other. For the sake of completeness we should like to take up once more the question of the influence of statistical fluctuations on the time τ it takes for the system to move from saddle to scission. In [5] the following formula had been derived, based

on Kramers' equation:

$$\tau = \frac{\tau_0}{\sqrt{1+\eta^2}-\eta} \equiv \frac{2\mathcal{R}(\sqrt{M\varpi^2 q_{sc}^2/2T})}{\varpi(\sqrt{1+\eta^2}-\eta)} \tag{14}$$

with $\mathcal{R}(x)$ being the Rosser function

$$\mathcal{R}(x) = \int_0^x \exp(y^2)dy \int_y^\infty \exp(-z^2)dz \tag{15}$$

In the quantum case the argument of the $\mathcal{R}$ in (14) would get the additional factor $\sqrt{T/C\Sigma_{qq}^{\mathrm{eq}}}$ [3], but as can be seen from Fig.2 of this reference this modification may safely be neglected for $T/\hbar\varpi > 0.5$. For that regime Fig.5 shows the $\varpi\tau_0$ as function of $\Delta V/T = M\varpi^2 q_{sc}^2/2T$. As the $\hbar\varpi$ is of the order of 1 MeV, the τ_0 is seen to lie in the range of $1 \; - \; 2 \times 10^{-21}$s.

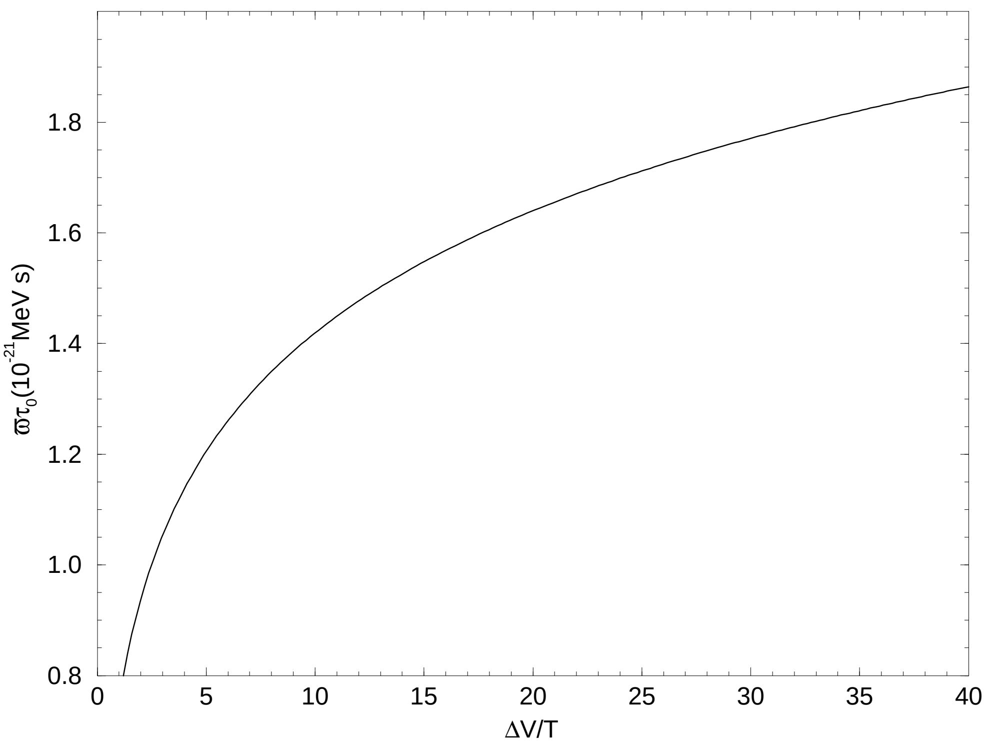

Figure 5: The mean saddle-to-scission time τ_0 (scaled by ϖ) as function of the difference ΔV of the potential energy (measured in units of T).

It is interesting to compare the result (14) with the one one would get if the system would move along a trajectory starting on top of the barrier with the momentum P_0 (i.e. including disipation but discarding the fluctuating force). As seen from (13) one gets a formula like (14) but with the $2\mathcal{R}(\sqrt{M\varpi^2 q_{sc}^2/2T})$ replaced by $\ln(2M\varpi q_{sc}\sqrt{1+\eta^2}/P_0)$. To make the analogy to (14) even closer one may estimate the initial momentum by associating $P_0^2/2M$ to an average, thermal kinetic energy on top of the barrier. One might be tempted to use for the

latter $E_{\text{kin}} = T/2$, the value given by the equipartition theorem. A numerical evaluation shows that in this case one would overestimate the τ_0 by about 10% (for $\eta = 1$) to 50 % (for $\eta = 10$). However, as we may learn from (11), for the inverted oscillator the stationary solution suggests a larger value of the average kinetic energy. Putting there the $q_{sc} = 0$ one obtains (in the high-T limit) $E_{\text{kin}} = T(1 + \eta\zeta)$, which for zero damping gives twice the value of the equipartition theorem. This modification would improve the results slightly.

Finally, we wish to add some remarks on the variation with q. It is evident from the discussion given above that under certain circumstances the Kramers-Ingold solution may be applied for regions before scission. It may thus be used for performing averages over quantities which simply depend on the collective variable. Prime examples are the evaporation probabilities for light particles [21] and γ-rays (see [17]). Adopting the same normalization as in (7, 8) one gets as weighting factor the current j which according to (9) is constant. This implies that for the motion from saddle to scission an average in the coordinate q simply reduces to the algebraic one.

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